Author index to volume 63

Almeida, R., see C.E. Dateo 63 (1991) 435

Baer, M., see D. Neuhauser 63 (1991) 460
Balakrishnan, N. and N. Sathyamurthy, Time-dependent wave-packet methods for the calculation of collinear atom–diatom exchange reaction probabilities 63 (1991) 209
Balint-Kurti, G.G., R.N. Dixon, C.C. Marston and A.J. Mulholland, The calculation of product quantum state distributions and partial cross-sections in time-dependent molecular collision and photodissociation theory 63 (1991) 126
Berger, J.F., M. Girod and D. Gogny, Time-dependent quantum collective dynamics applied to nuclear fission 63 (1991) 365
Berman, M. and R. Kosloff, Time-dependent solution of the Liouville–von Neumann equation: non-dissipative evolution 63 (1991) 1
Berne, B.J., see D. Thirumalai 63 (1991) 415
Besprozvannaya, A. and D.J. Tannor, Fast sine/cosine transform for periodic functions with reflection symmetry 63 (1991) 569
Billing, G.D., Basis set independent methods in time-dependent dynamics 63 (1991) 38
Bottcher, C., G.J. Bottrell and M.R. Strayer, Time-dependent Hartree–Fock studies of atomic collisions 63 (1991) 63
Bottrell, G.J., see C. Bottcher 63 (1991) 63

Cerjan, C. and K.C. Kulander, Efficient time propagation for finite-difference representations of the time-dependent Schrödinger equation 63 (1991) 529
Cerjan, Ch., see P. Pernot 63 (1991) 259
Chu, S.-I. and T.-F. Jiang, Nonperturbative methods for the study of multiphoton dynamics in intense periodic and multi-color laser fields 63 (1991) 482

Dateo, C.E., V. Engel, R. Almeida and H. Metiu, Numerical solutions of the time-dependent Schrödinger equation in spherical coordinates by Fourier transform methods 63 (1991) 435
DeVries, P.L., The time evolution of the hydrogen wavefunction in intense laser fields 63 (1991) 95
Dixon, R.N., see G.G. Balint-Kurti 63 (1991) 126
Dreizler, R.M., see H.J. Lüdde 63 (1991) 345

Engel, V., Excitation of molecules with ultrashort laser pulses: exact time-dependent quantum calculations 63 (1991) 228
Engel, V., see C.E. Dateo 63 (1991) 435

Faisal, F.H.M. and P. Scanzano, Solution of the initial value-problem in laser–atom interaction: a variational Fourier transform method 63 (1991) 265
Friesner, R.A., see F. Webster 63 (1991) 494

Garcia, J.D., see N.H. Kwong 63 (1991) 171
Garcia, J.D., see K.J. Shafer 63 (1991) 306
Gauss, J. and E.J. Heller, A time-dependent semiclassical wave-packet method using a fast Fourier transform (FFT) algorithm 63 (1991) 375
Girod, M., see J.F. Berger 63 (1991) 365
Gogny, D., see J.F. Berger 63 (1991) 365
Grün, N., see P. Zimmerer 63 (1991) 21

Heather, R.W., An asymptotic wavefunction splitting procedure for propagating spatially extended wavefunctions: application to intense field photodissociation of H_2^+ 63 (1991) 446
Heller, E.J., see J. Gauss 63 (1991) 375
Hooper Jr., C.F., see R.C. Mancini 63 (1991) 314
Horbatsch, M., A semiclassical independent electron model for ion–atom collisions 63 (1991) 115
Humbert, J., see G. Jolicard 63 (1991) 216

Iung, C. and C. Leforestier, Exact time evolution methods for large bound systems 63 (1991) 135

Jackson, B., Time-dependent mean-field approach to molecule–surface scattering at finite temperatures 63 (1991) 154
Jiang, T.-F., see S.-I. Chu 63 (1991) 482
Jolicard, G. and J. Humbert, Stationary and time-dependent wave-operator formulation in molecular dynamics 63 (1991) 216
Judson, R.S., see D. Neuhauser 63 (1991) 460

Kilcrease, D.P., see R.C. Mancini 63 (1991) 314
Kosloff, R., see M. Berman 63 (1991) 1
Kotler, Z., E. Neria and A. Nitzan, Multiconfiguration time-dependent self-consistent field approximations in the numerical solution of quantum dynamical problems 63 (1991) 243
Kouri, D.J., see Y. Sun 63 (1991) 51
Kouri, D.J., see R.C. Mowrey 63 (1991) 100
Kouri, D.J., see D. Neuhauser 63 (1991) 460
Kulander, K.C., see D.H. Tiszauer 63 (1991) 351
Kulander, K.C. and T.N. Rescigno, Effective potentials for time-dependent calculations of multiphoton processes in atoms 63 (1991) 523
Kulander, K.C., see C. Cerjan 63 (1991) 529
Kwong, N.H., K.J. Schaudt and J.D. Garcia, Solution of quantum evolution equations by finite-difference 63 (1991) 171
Kwong, N.H., see K.J. Shafer 63 (1991) 306

Leforestier, C., see C. Iung 63 (1991) 135
Lester Jr., W.A., see P. Pernot 63 (1991) 259
Lin, F.J. and J.T. Muckerman, Solution of the time-dependent Schrödinger equation employing a basis of explicit discrete-coordinate eigenfunctions: spherical and azimuthal symmetry, adiabaticity, and multiphoton excitation of a rotating Morse oscillator 63 (1991) 537
Lüdde, H.J. and R.M. Dreizler, Microscopic optical potentials for time-dependent quantum systems 63 (1991) 345

Makri, N., Feynman path integration in quantum dynamics 63 (1991) 389
Mancini, R.C., D.P. Kilcrease, L.A. Woltz and C.F. Hooper Jr., Calculation aspects of the Stark line broadening of multi-electron ions in plasmas 63 (1991) 314
Marston, C.C., see G.G. Balint-Kurti 63 (1991) 126
McCurdy, C.W. and C.K. Stroud, Eliminating wave-packet reflection from grid boundaries using complex coordinate contours 63 (1991) 323
Metiu, H., see C.E. Dateo 63 (1991) 435
Micha, D.A., see D. Srivastava 63 (1991) 331
Mickens, R.E., Novel explicit finite-difference schemes for time-dependent Schrödinger equations 63 (1991) 203
Mowrey, R.C. and D.J. Kouri, Inelastic molecule-corrugated surface scattering using the close-coupling wave-packet method 63 (1991) 100
Muckerman, J.T., see F.J. Lin 63 (1991) 537
Mulholland, A.J., see G.G. Balint-Kurti 63 (1991) 126

Neria, E., see Z. Kotler 63 (1991) 243
Neuhauser, D., M. Baer, R.S. Judson and D.J. Kouri, The application of time-dependent wavepacket methods to reactive scattering 63 (1991) 460
Nitzan, A., see Z. Kotler 63 (1991) 243

Pernot, P., W.A. Lester Jr. and Ch. Cerjan, Quantum time-dependent treatment of molecular collisions: scattering of He by $H_2(B^1(\Sigma_u^+)$ 63 (1991) 259

Rabitz, H., see S. Shi 63 (1991) 71
Rescigno, T.N., see K.C. Kulander 63 (1991) 523
Richardson, J.L., Visualizing quantum scattering on the CM-2 supercomputer 63 (1991) 84
Rossky, P.J., see F. Webster 63 (1991) 494

Sathyamurthy, N., see N. Balakrishnan 63 (1991) 209
Scanzano, P., see F.H.M. Faisal 63 (1991) 265
Schafer, K.J., The energy analysis of time-dependent numerical wave functions 63 (1991) 427
Schaudt, K.J., see N.H. Kwong 63 (1991) 171
Scheid, W., see P. Zimmerer 63 (1991) 21
Schwenke, D.W., see Y. Sun 63 (1991) 51
Shafer, K.J., N.H. Kwong and J.D. Garcia, Development of B-spline techniques for dynamic ion–metal interaction theories 63 (1991) 306
Shi, S. and H. Rabitz, Optimal control of bond selectivity in unimolecular reactions 63 (1991) 71
Skodje, R.T., see A. Spina 63 (1991) 279
Spina, A. and R.T. Skodje, The phase-space hydrodynamic model for the quantum standard map 63 (1991) 279
Srivastava, D. and D.A. Micha, Complex-time path-integration with time-dependent Hamiltionans for extended molecular systems 63 (1991) 331
Strayer, M.R., see C. Bottcher 63 (1991) 63
Strayer, M.R., see A.S. Umar 63 (1991) 179
Stroud, C.K., see C.W. McCurdy 63 (1991) 323
Sun, Y., D.J. Kouri, D.W. Schwenke and D.G. Truhlar, Time-dependent wave-packet algorithm for inelastic molecule–molecule scattering 63 (1991) 51

Tannor, D.J., see A. Besprozvannaya 63 (1991) 569
Thirumalai, D. and B.J. Berne, Methods for simulating time correlation functions in quantum systems 63 (1991) 415
Tiszauer, D.H. and K.C. Kulander, Computation methods employed in the self-consistent time-dependent, Hartree–Fock calculation for a reactive molecular collision 63 (1991) 351
Truhlar, D.G., see Y. Sun 63 (1991) 51

Umar, A.S. and M.R. Strayer, Numerical methods for nuclear mean-field dynamics 63 (1991) 179

Webster, F., P.J. Rossky and R.A. Friesner, Nonadiabatic processes in condensed matter: semi-classical theory and implementation 63 (1991) 494
Woltz, L.A., see R.C. Mancini 63 (1991) 314

Zhang, J.Z.H., Multichannel quantum wave-packet propagation in the interaction picture: application to gas–surface scattering 63 (1991) 28
Zimmerer, P., M. Zimmermann, N. Grün and W. Scheid, Trajectory method for the time-dependent Schrödinger and Thomas–Fermi equations 63 (1991) 21
Zimmermann, M., see P. Zimmerer 63 (1991) 21

Subject index to volume 63

above-threshold detachment 265
above-threshold ionization (ATI) 95, 427
absorbing potentials 460
adiabatic dynamics 415
autocorrelation funtions 95

basis-spline collocation method 63, 179, 306
bond selectivity 71

chaos 279
charge transfer 351
Chebycheff, Chebychev, Chebyshev 1, 100, 529
close-coupling wave packet method 28, 51, 100, 460
CM-2 supercomputer 84
complex coordinates 323
complex-time path-integration 331
Cranck–Nicolson 171

discrete variable representation 203

effective potentials 523

fast Fourier transform (FFT) 1, 51, 71, 95, 100, 209, 243, 435, 482, 529, 569
Feshbach formalism 345
Feynman path integral 331, 389, 415
final state distributions 51, 228
finite difference 95, 171, 203, 209, 351, 529
Floquet expansion 265, 482

gas–surface scattering 28, 154

harmonic generation 523
Hartree–Fock 63, 351
heavy-ion collisions 63, 171
hydrodynamic model 279

impact-parameter approximation 115
inelastic molecule–molecule scattering 51
infrared spectra 135
intense laser fields 265, 446
intramolecular vibrational relaxation 135
ion–atom collisions 115, 345
ion–surface scattering 306

Lanczos 435, 494
laser–atom interactions 21, 523
Lippmann–Schwinger equation 51

mean-field approximations 38
molecular collisions 51
molecular dynamics 216
molecular photodissociation 126, 228, 331, 446
molecular photodissociaton 375
molecule–surface scattering 100
Monte Carlo 389
multi-channel quantum wave packets 51
multi-photon processes 482, 523
multiple ionization 115

non-adiabatic transitions 243, 494
nuclear dynamics 179, 365
nuclear fission 365

optical potentials 345

parallelization 135
projection operators 216, 345
propagation methods 51, 84, 529, 538
proton–hydrogen scattering 21

quantum standard map 279

reactive scattering 126, 209, 460

self-consistent field methods 365
semiclassical methods 375, 389, 494
short-pulse laser excitation 228, 538
spectral method 95, 435, 569
split operator 84, 95, 375
splitting method 71, 84, 259, 446
Stark line broadening 314
surface hopping 494

time-dependent Hartree–Fock (TDHF) 179
time-dependent Schrödinger equation 21
time-dependent self-consistent field (TDSCF) 38, 115, 154, 243, 331
time-dependent Thomas–Fermi equation 21
trajectory method 21

Vlasov equation 115

wave packet 38, 51, 126, 154, 209, 259, 323, 460, 538
window function 427